

A physical application of g -function

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We investigated an integral representation of a complex function which was obtained from the molecular beam magnetic resonance, and named it as ' g -function' because it was connected with Gamma function as a special case. We introduced a physical example of the g -function from a dipole-dipole interaction of rigid polar molecules.

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Quantum mechanics cannot stand without special functions such as Bessel function or Legendre function. Besides these functions, there are so many functions that was originated from mathematics but has been used in physical sciences more than mathematics. On the other hand there are still many functions that has been studied by mathematician but has been rarely used in other areas. Among them some functions do not have even names.

In this paper, we will introduce a mathematical function which has not name yet and has been considered as no physical application. We call it as g -function because the gamma function is a very special case of the function. Of course it is totally different from the generalized or modified Gamma functions. We'll use small ' g ' to avoid the confusion from the Meijer's G -function [1]. Then, we will introduce a physical example of the typical case of the g -function. from a familiar classical model of an electromagnetic theory.

In various theoretical physics such as a neutron beam velocity distribution function [2, 3] or a theory of the molecular beam magnetic resonance method [4, 5, 6], there arise a definite integral function $\int_0^\infty y e^{-y^2 - z/y} dy$, where z is a complex number. It was the birth of a new complex function containing the Gamma function as a special case.

In 1937 the g -function was introduced by Zahn [2] from an absorption coefficients for slow thermal neutrons. The fraction of neutrons transmitted is given by

$$\phi_1(x) = \int_0^\infty y e^{-y - x/y^{1/2}} dy. \quad (1)$$

Then, the function was extended to m -th order by Laporte [3]. The extended form was given by

$$\phi_m(x) = \int_0^\infty y^m e^{-y - x/y^{1/2}} dy. \quad (2)$$

The order m is restricted to positive integer here. He showed that the integral function is a solution of a third-order linear differential equations. Also the convergent expansions were obtained for small values of x .

Later in 1941 the modern form of the m -th order g -function was introduced by Torrey [5] in a neutron beam velocity distribution. The transition probability in radio-frequency spectra contains the function. At result in 1951 the 3rd order g -function was studied mathematically by Kruse and Ramsey [7]. At this time the g -function was extended into complex plane.

The complete form of the m -th order g -function is defined by

$$g_m(z) = \int_0^\infty y^m e^{-y^2 - z/y} dy, \quad (3)$$

where $m = 0, 1, 2, \dots$, and z is a complex number. Interchanging y into $1/x$, we obtain another expression of $g_m(z)$ as

$$g_m(z) = \int_0^\infty \frac{e^{-1/x^2 - zx}}{x^{m+2}} dx. \quad (4)$$

Therefore, the Gamma function is a special case of the g -function as

$$g_m(0) = \frac{1}{2} \Gamma\left(\frac{m+1}{2}\right). \quad (5)$$

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Alternatively,

$$g_{2m+1}(0) = \frac{n!}{2}. \quad (6)$$

The g_m has the following three fundamental properties [8]. First, it is a solution of the 3rd order differential equation

$$x \frac{d^3 g_m}{dx^3} - (m-1) \frac{d^2 g_m}{dx^2} + 2g_m(x) = 0, \quad (7)$$

where $m = 0, 1, 2, \dots$. Second, the derivative reduces single order and change its sign

$$\frac{dg_m}{dx} = -g_{m-1}(x), \quad (8)$$

where $m = 1, 2, 3, \dots$. Third, it satisfies the recurrence relation

$$2g_m(x) = (m-1)g_{m-2}(x) + xg_{m-3}(x), \quad (9)$$

where $m = 3, 4, 5, \dots$. More basic properties of the g_m in pure mathematical aspects are summarized in the handbook by Abramowitz and Stegun [8].

The $g_m(z)$ can be also written as $g_m(r, \theta)$ in the polar coordinate. The complex z is written as $z = re^{-i\theta}$, where $r = |z|$ and $0 \leq \theta \leq \pi/2$. Then, the real and imaginary parts are

$$Reg_m(r, \theta) = \int_0^\infty y^m e^{-y^2 - \frac{r \cos \theta}{y}} \cos\left(\frac{r \sin \theta}{y}\right) dy, \quad (10)$$

and

$$Img_m(r, \theta) = \int_0^\infty y^m e^{-y^2 - \frac{r \cos \theta}{y}} \sin\left(\frac{r \sin \theta}{y}\right) dy. \quad (11)$$

It oscillates very slowly around r axis but converges to zero quickly.

Furthermore, $g_m(z)$, $m = 0, 1, 2, \dots$, does not have infinite Taylor series expansion because it is expanded up to the m -th order of z at $z = 0$. From Eqs. (4) and (8) the n -th derivatives of $g_m(z)$ by z is

$$\frac{d^n g_m(z)}{dz^n} = (-1)^n \int_0^\infty \frac{e^{-1/x^2 - zx}}{x^{m-n+2}} dx. \quad (12)$$

where $n \geq 1$. If we check the value at the origin,

$$\begin{aligned} \lim_{|z| \rightarrow 0} \frac{d^n g_m(z)}{dz^n} &= \text{finite constant} : n \leq m. \\ &= \text{infinite} : n > m. \end{aligned} \quad (13)$$

Although it has some possibilities of exciting features, there has been no more serious studies in the g_m function since 1950s. The main reason is that the application area of the function has never been found besides the previous known fields. Furthermore, the function was not considered seriously as an extended form of the Gamma function. That is, the further studies of the g_m was retarded by the restriction of the application area even though it has many interesting properties.

We introduce a classical example of the $g_1(z)$ in a complex plane. It comes from the Fourier transformation of the time correlation function of dipoles in linear response theory. We begin our story of the function from an example: the frequency dependent electric susceptibility of polar molecules.

We assume a homogeneous isotropic fluid of rigid particles. In general the shape of a rigid molecule is arbitrary, and has three different moment of inertia. Also we assume that it has a dipole moment $\mu(t)$ in the direction of rotating axis. Let ω be the applied frequency and τ be a relaxation time by collision of the rotating particles. Then, the self part of the electric susceptibility has the following form [9, 10, 11, 12].

$$\frac{\chi_s(\omega + i/\tau)}{\chi_s(0)} = 1 + i(\omega + i/\tau) \int_0^\infty e^{i(\omega + i/\tau)t} \frac{\langle \mu(0) \cdot \mu(t) \rangle}{\mu^2} dt. \quad (14)$$

$\langle \dots \rangle$ denotes an ensemble average over initial conditions or the statistical average in the absence of applied fields.

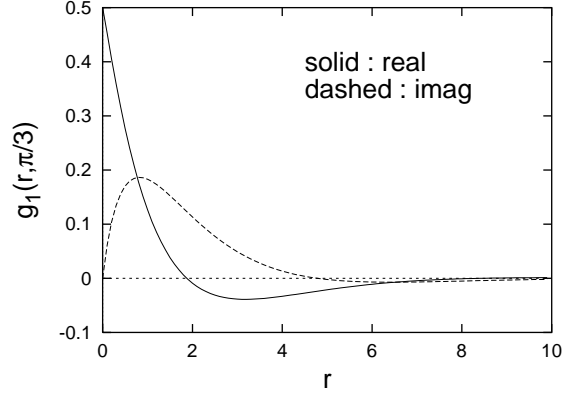


FIG. 1: The radial dependence of $g_1(r, \pi/3)$.

Let $(\theta_i(t), \phi_i(t), \psi_i(t))$ be the Euler angles that describe the orientation of particle i at time t with respect to a laboratory fixed frame of reference. Also, let I_i and Ω_i ($i = 1, 2, 3$) be the moment of inertia and angular velocity of the three dimensional rigid body to its three principal axes. Then, the angular momentum L_i satisfies $L_i = I_i \Omega_i$. The kinetic energy of an arbitrary shape of rotating three dimensional rigid body is composed of translational and rotational motion. That is,

$$\begin{aligned} E &= \frac{P^2}{2M} + \frac{1}{2} \sum_{i=1}^3 I_i \Omega_i^2 \\ &= \frac{P^2}{2M} + \frac{f(\theta, \psi) L^2}{2I_3}, \end{aligned} \quad (15)$$

where M is the mass and P is the linear momentum. The $f(\theta, \psi)$ is the angular momentum relation function that is defined by

$$f(\theta, \psi) = \frac{I_3}{I_1} \sin^2 \theta \sin^2 \psi + \frac{I_3}{I_2} \sin^2 \theta \cos^2 \psi + \cos^2 \theta. \quad (16)$$

$f(\theta, \psi)$ varies *smoothly* in θ and ψ , and it gives us the relation between the rotational kinetic energy and the angular momentum. The translational motion of the particle gives just a constant in calculation of the statistical average. Therefore, we can neglect $P^2/2M$ term in further steps.

For convenience we define the angle difference of the dipole μ at time 0 and t as γ . Then, we can write the dipole-dipole correlation function in Eq. (14) as

$$\frac{\mu(0) \cdot \mu(t)}{\mu^2} = \cos \gamma(\theta, \psi, u), \quad (17)$$

where u is a dimensionless time defined by $u = Lt/I_3$. This conversion makes the $\cos \gamma$ not include L explicitly.

Applying Eqs. (15) and (17) to Eq. (14) produces $g(\theta, \psi, u)$ as an essential part of the Fourier transformation.

$$\frac{\chi_s(\omega + i/\tau)}{\chi_s(0)} = 1 + \frac{i(\omega + i/\tau)}{Z} \int_0^\infty du \int_0^\pi \sin \theta d\theta \int_0^{2\pi} \cos \gamma(\theta, \psi, u) g(\theta, \psi, u) d\psi, \quad (18)$$

where

$$g(\theta, \psi, u) = \int_0^\infty L e^{-(\beta f/2I_3)L^2 - (1/\tau - i\omega)I_3 u/L} dL. \quad (19)$$

The Z is the partition function and independent of the initial position and time. $\beta = 1/k_B T$, where k_B is the Boltzmann constant and T is the absolute temperature.

Eventually, the integral expression of $g(\theta, \psi, u)$ is directly related with the $g_1(z)$ in complex plane as

$$g_1(z) = \int_0^\infty y e^{-y^2 - z/y} dy. \quad (20)$$

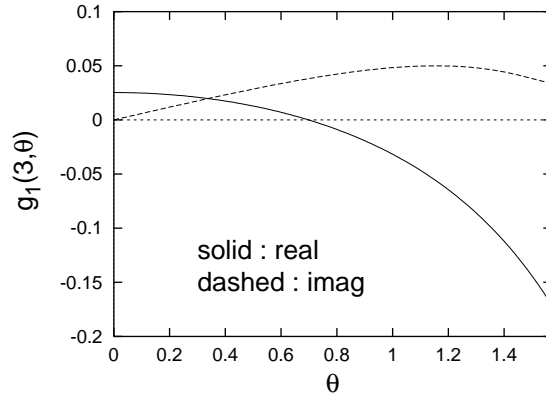


FIG. 2: The phase dependence of $g_1(3, \theta)$.

The z is a complex number given by $z = z_1 - iz_2$. Comparing Eq. (18) with Eq. (19), the regions of the real number z_1 and z_2 are decided as $z_1 > 0$, and $z_2 > 0$. We plotted the real and imaginary parts of the $g_1(r, \theta)$. The radial dependence at $\theta = \pi/3$ was plotted in FIG. 1, and we see that it oscillates and quickly drops to zero. The phase dependence at $r = 3$ is plotted in FIG. 2, too.

We named a special function as g_m function with order m , and studied some fundamental properties of it. A physical example of the g -function in a complex plane was introduced from classical mechanics and electromagnetic theory.

Although, some functions has been regarded as not useful application areas, it is not actually true. We have not found the application area yet. It is interesting enough to study connecting with the Gamma function. Merging to 0 of the radial part is quicker than Bessel functions and Neumann functions, and that may applicable to a new integral transformation. We hope that it covers various range of physics that previous ordinary Gamma function could not.

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